

125487

SEARCH REQUEST FORM

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Shear

Scientific and Technical Information Center

Requester's Full Name: C. Delacruz Examiner #: 71100 Date: 6-22-00
Art Unit: 1614 Phone Number: 202-272-0572 Serial Number: 091825, 989
Mail Box and Bldg Room Location: 4C85 (coffee) 4C70 (mail box) Results Format Preferred (circle): PAPER DISK FAX
If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the chemical species, structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept of the invention. Define any terms that may have a special meaning. Give examples of relevant citations, authors, etc. known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____
Inventors (please provide full names): _____
Earliest Priority Filing Date: _____
PLEASE SEE ATTACHED

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search claims 45 + 58.
Key terms are highlighted.

Rush Search Approval

SPF, AC 16-15

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Please rush - Than

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Type of Search

Vendors and cost where applicable

Searcher

NA Sequence (#)

STN

09/825989

FILE 'REGISTRY' ENTERED AT 12:07:49 ON 24 JUN 2004
 E ISOTHIOCYANATE/CN 5
 L1 1 SEA ABB=ON PLU=ON ISOTHIOCYANATE/CN
 E GLUCOSINOLATE/CN 5
 E MYROSINASE/CN 5
 L2 1 SEA ABB=ON PLU=ON MYROSINASE/CN

FILE 'CAPLUS' ENTERED AT 12:08:58 ON 24 JUN 2004
 L3 32844 SEA ABB=ON PLU=ON L1 OR ISOTHIOCYANATE OR ISO(W) (THIOCY
 ANATE OR THIO CYANATE) OR ISOTHIO CYANATE OR GLUCOSINOLAT
 E
 L4 515 SEA ABB=ON PLU=ON L3 AND (L2 OR MYROSINASE)

FILE 'REGISTRY' ENTERED AT 12:10:50 ON 24 JUN 2004
 E DIMETHYLSULFOXIDE/CN 5
 E DIMETHYL SULFOXIDE/CN 5
 L5 1 SEA ABB=ON PLU=ON "DIMETHYL SULFOXIDE"/CN
 E ACETONITRILE/CN 5
 L6 2 SEA ABB=ON PLU=ON (ACETONITRILE/CN OR "ACETONITRILE
 (13CH3CN)"/CN)
 E DIMETHYLFORMAMIDE/CN 5
 L7 1 SEA ABB=ON PLU=ON DIMETHYLFORMAMIDE/CN

FILE 'CAPLUS' ENTERED AT 12:11:31 ON 24 JUN 2004
 L8 0 SEA ABB=ON PLU=ON L4 AND (L5 OR DIMETHYLSULFOXIDE OR
 DIMETHYLSULPHOXIDE OR DI(W) (METHYLSULFOXIDE OR METHYLSULP
 HOXIDE OR (ME OR METHYL) (W) (SULFOXIDE OR SULPHOXIDE)) OR
 DIMETHYL(W) (SULFOXIDE OR SULPHOXIDE))
 L9 12 SEA ABB=ON PLU=ON L4 AND (L6 OR ACETONITRILE OR ACETO
 NITRILE)
 L10 1 SEA ABB=ON PLU=ON L4 AND (L7 OR DIMETHYLFORMAMIDE OR
 DI(W) (METHYLFORMAMIDE OR (ME OR METHYL) (W) FORMAMIDE) OR
 DIMETHYL FORMAMIDE)
 L11 12 SEA ABB=ON PLU=ON L9 OR L10

L11 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
 ED Entered STN: 26 Oct 2001
 ACCESSION NUMBER: 2001:780211 CAPLUS
 DOCUMENT NUMBER: 136:262229
 TITLE: Hydrolysis products of **glucosinolates**
 from white cabbage (*Brassica oleracea* L. var
capitata) and cauliflower (*Brassica oleracea* L.
 var *botrytis*) analyzed by HPLC and GC/MS
 AUTHOR(S): Delonga, Karmela; Smit, Zdenko; Dragovic-Uzelac,
 Verica; Mrkic, Vlatka; Vorkapic-Furac, Jasna
 CORPORATE SOURCE: Faculty of Food Technology and Biotechnology,
 University of Zagreb, Zagreb, HR-10000, Croatia
 SOURCE: Special Publication - Royal Society of Chemistry
 (2001), 269(Biologically-Active Phytochemicals
 in Food), 213-216
 CODEN: SROCDO; ISSN: 0260-6291
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB In this study the determination of **glucosinolates** (GSL) in cabbage
 and cauliflower, as well as their autolysis and hydrolysis products

obtained by exogenous enzyme **myrosinase** was performed by reversed-phase high performance liquid chromatog. (RP-HPLC) followed by gas-chromatog./mass spectrometry (GS/MS). The anal. data of the autolysis and hydrolysis products (pH 7.0) obtained by HPLC (DAD and FL detection) and GC/MS confirmed that their relationship depends on GSL precursors and conditions of their enzymic degradation (autolysis and hydrolysis). An examination of the indole GSL degradation products showed the presence of four to seven different compds. Three of them were identified as indole-3-carbinol (13C), indole-3-acetonitrile (13CN) and 3,3'-diindolylmethane (DIM).

IT 9025-38-1, **Myrosinase**

RL: BSU (Biological study, unclassified); BIOL (Biological study) (hydrolysis products of **glucosinolates** from white cabbage and cauliflower analyzed by HPLC and GC/MS)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

ED Entered STN: 28 Jun 2001

ACCESSION NUMBER: 2001:465523 CAPLUS

DOCUMENT NUMBER: 135:192989

TITLE: Jasmonate-dependent induction of indole **glucosinolates** in Arabidopsis by culture filtrates of the nonspecific pathogen *Erwinia carotovora*

AUTHOR(S): Brader, Gunter; Tas, Eva; Palva, E. Tapio

CORPORATE SOURCE: Department of Biosciences, University of Helsinki, Helsinki, FIN-00014, Finland

SOURCE: Plant Physiology (2001), 126(2), 849-860
CODEN: PLPHAY; ISSN: 0032-0889

PUBLISHER: American Society of Plant Physiologists

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Elicitors from the plant pathogen *Erwinia carotovora* trigger coordinate induction of the tryptophan (Trp) biosynthesis pathway and Trp oxidizing genes in Arabidopsis. To elucidate the biol. role of such pathogen-induced activation we characterized the production of secondary defense metabolites such as camalexin and indole **glucosinolates** derived from precursors of this pathway. Elicitor induction was followed by a specific increase in 3-indolylmethylglucosinolate (IGS) content, but only a barely detectable accumulation of the indole-derived phytoalexin camalexin. The response is mediated by jasmonic acid as shown by lack of IGS induction in the jasmonate-insensitive mutant *coi-1*. In accordance with this, Me jasmonate was able to trigger IGS accumulation in Arabidopsis. In contrast, ethylene and salicylic acid seem to play a minor role in the response. They did not trigger alterations in IGS levels, and Me jasmonate- or elicitor-induced IGS accumulation in *NahG* and ethylene-insensitive *ein2-1* mutant plants was similar as in the wild type. The breakdown products of IGS and other **glucosinolates** were able to inhibit growth of *E. carotovora*. The results suggest that IGS is of importance in the defense against bacterial pathogens.

IT 9025-38-1, **Myrosinase**

RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); BIOL (Biological study)
 (jasmonate-dependent induction of indole **glucosinolates**
 in Arabidopsis by culture filtrates of the nonspecific pathogen
 Erwinia carotovora)

REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L11 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

ED Entered STN: 08 Jun 1999

ACCESSION NUMBER: 1999:350134 CAPLUS

DOCUMENT NUMBER: 131:127727

TITLE: Induction of auxin biosynthetic enzymes by
 jasmonic acid and in clubroot diseased Chinese
 cabbage plants

AUTHOR(S): Grsic, Slobodanka; Kirchheim, Brigitte; Pieper,
 Kerstin; Fritsch, Monika; Hilgenberg, Willy;
 Ludwig-Muller, Jutta

CORPORATE SOURCE: Botanisches Institut, Johann Wolfgang
 Goethe-Universitat, Frankfurt, D-60054, Germany

SOURCE: Physiologia Plantarum (1999), 105(3), 521-531
 CODEN: PHPLAI; ISSN: 0031-9317

PUBLISHER: Munksgaard International Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Nitrilase (NIT) and **myrosinase** are important enzymes for
 auxin biosynthesis in Brassicaceae, synthesis which is increased
 during clubroot disease. Therefore, NIT and **myrosinase**
 levels during club development and possible regulation mechanisms
 were investigated. In addition, the occurrence of different nitrilase
 isoforms in Chinese cabbage has been shown. Nitrilase activity was
 enhanced in infected roots during later stages of club development
 (35-42 days after inoculation). However, no differences in
 nitrilase mRNA levels between infected and healthy roots were found
 during symptom development. **Myrosinase** expression was
 increased in clubbed roots at slightly earlier time points (28 days
 after inoculation) and also at later time points during infection.
 The activities of tryptophan-oxidizing enzyme (TrpOxE), which
 catalyzes the first step in tryptophan-dependent auxin biosynthesis
 in Brassicaceae, and nitrilase were enhanced after treatment with
 jasmonic acid (JA) and Me jasmonate. Similarly, the amount of
myrosinase mRNA was increased by JA. During clubroot
 disease the endogenous concentration of JA increased in infected roots 3-5
 wk after inoculation. From these results it can be concluded that:
 (1) de novo indole-3-acetic acid (IAA) biosynthesis plays a role for
 symptom development of clubroot disease in Brassicaceae during later
 developmental stages; and (2) JA, which increased during club
 development, may be involved in the up-regulation of three enzymes
 important for IAA synthesis.

IT 9025-38-1, **Myrosinase**

RL: BSU (Biological study, unclassified); MFM (Metabolic formation);
 BIOL (Biological study); FORM (Formation, nonpreparative)
 (induction of auxin-forming enzymes in Chinese cabbage plants by
 jasmonic acid and in clubroot disease)

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE

09/825989

IN THE RE FORMAT

L11 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
ED Entered STN: 29 Jan 1999
ACCESSION NUMBER: 1999:61408 CAPLUS
DOCUMENT NUMBER: 130:167342
TITLE: Development of a new method for the evaluation
of heavy volatile **glucosinolate**
decomposition products
AUTHOR(S): Froehlich, G.; Fingerling, G.; Hanke, A.; He,
H.; Schnitzler, W. H.
CORPORATE SOURCE: TU Munich, Freising-Weiherstephan, D-85350,
Germany
SOURCE: Lebensmittelchemie (1999), 53(1), 5-6
CODEN: LEBEE2; ISSN: 0937-1478
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: German
AB A new method was developed for the enrichment of heavy volatile
glucosinolate decomposition products. **Glucosinolates**
were separated from (Brassica oleracea convar. acephala var. sabellica)
after deactivation of the **myrosinase** and were metabolized
by addition of external **myrosinase**. The identification of
the **glucosinolate** decomposition products was performed by
GC/MS. A great influence of the pH during incubation was noticed.
The broadest spectrum of decomposition products was found when the pH was
equal to the vegetable extract (pH=5.8). 2-Propenyl-ITC,
2-phenylethyl-ITC, 1-cyano-2,3-epithiopropion, and
3-indolylmethylcyanide were detected at every pH. Independent of
the pH during incubation, 5-vinylloxazolidin-2-thione,
3-methylthiopropyl-ITC, and 3-indolylmethylcyanide were detectable for
the 1st time.
IT **9025-38-1, Myrosinase**
RL: ARG (Analytical reagent use); BSU (Biological study,
unclassified); ANST (Analytical study); BIOL (Biological study);
USES (Uses)
(determination of heavy volatile **glucosinolate** decomposition
products in kale)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN
THE RE FORMAT

L11 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
ED Entered STN: 31 Oct 1997
ACCESSION NUMBER: 1997:687616 CAPLUS
DOCUMENT NUMBER: 127:277421
TITLE: Enzymic, Chemical, and Thermal Breakdown of
3H-Labeled Glucobrassicin, the Parent Indole
Glucosinolate
AUTHOR(S): Chevolleau, Sylvie; Gasc, Nicole; Rollin,
Patrick; Tulliez, Jacques
CORPORATE SOURCE: Laboratoire des Xenobiotiques, INRA, Toulouse,
31931, Fr.
SOURCE: Journal of Agricultural and Food Chemistry
(1997), 45(11), 4290-4296
CODEN: JAFCAU; ISSN: 0021-8561

Searcher : Shears 571-272-2528

09/825989

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The enzymic, chemical, and thermal breakdown pathways of glucobrassicin, the major indolylmethyl **glucosinolate** of cruciferous vegetables, have been studied using synthetic 3H-labeled glucobrassicin (GBS). Radio-HPLC was used to analyze qual. and quant. the resulting products as well as their kinetics of formation. Enzymic breakdown of GBS under **myrosinase** action gave rise to different indole compds. [indole-3-carbinol (I3C), indole-3-**acetonitrile** (IAN), and 3,3'-diindolylmethane (DIM)]. At neutral pH, GBS degradation was almost complete after 1 h, and the major breakdown product was I3C, which could be converted to DIM. The formation of this self-condensation product was observed as photosensitive. In acidic conditions, enzymic degradation of GBS was a slower phenomenon, requiring 24 h to be nearly complete. IAN and I3C were the only 2 products occurring, and it was observed that the light had no effect either on the rate of formation or on the relative proportions of the breakdown products observed. GBS appeared as a very stable compound since no chemical degradation could be observed after 2 h in different aqueous media with pH in the 2-11 range. Moreover, after exposure to heat treatment, GBS was weakly degraded (10% in 1 h), giving rise to a new minor indole condensation product corresponding to a 3-indolylmethylglucobrassicin (IM-GBS).

IT **9025-38-1, Myrosinase**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(enzymic and chemical and thermal breakdown of 3H-labeled glucobrassicin, parent indole **glucosinolate**)

L11 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

ED Entered STN: 01 Oct 1997

ACCESSION NUMBER: 1997:625038 CAPLUS

DOCUMENT NUMBER: 127:292314

TITLE: Broccoli sprouts: an exceptionally rich source of inducers of enzymes that protect against chemical carcinogens

AUTHOR(S): Fahey, Jed W.; Zhang, Yuesheng; Talalay, Paul
CORPORATE SOURCE: Brassica Chemoprotection Laboratory and Department of Pharmacology and Molecular Sciences, The Johns Hopkins University School of Medicine, Baltimore, MD, 21205, USA

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1997), 94(19), 10367-10372

CODEN: PNASA6; ISSN: 0027-8424

PUBLISHER: National Academy of Sciences

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Induction of phase 2 detoxication enzymes [e.g., glutathione transferases, epoxide hydrolase, NAD(P)H: quinone reductase, and glucuronosyltransferases] is a powerful strategy for achieving protection against carcinogenesis, mutagenesis, and other forms of toxicity of electrophiles and reactive forms of oxygen. Since

Sept. 16
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prior
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Searcher : Shears 571-272-2528

consumption of large quantities of fruit and vegetables is associated with a striking reduction in the risk of developing a variety of malignancies, it is of interest that a number of edible plants contain substantial quantities of compds. that regulate mammalian enzymes of xenobiotic metabolism. Thus, edible plants belonging to the family Cruciferae and genus Brassica (e.g., broccoli and cauliflower) contain substantial quantities of **isothiocyanates** (mostly in the form of their **glucosinolate** precursors) some of which (e.g., sulforaphane or 4-methylsulfinylbutyl **isothiocyanate**) are very potent inducers of phase 2 enzymes. Unexpectedly, 3-day-old sprouts of cultivars of certain crucifers including broccoli and cauliflower contain 10-100 times higher levels of glucoraphanin (the **glucosinolate** of sulforaphane) than do the corresponding mature plants. **Glucosinolates** and **isothiocyanates** can be efficiently extracted from plants, without hydrolysis of **glucosinolates** by **myrosinase**, by homogenization in a mixture of equal vols. of DMSO, **DMF**, and **acetonitrile** at -50°C. Exts. of 3-day-old broccoli sprouts (containing either glucoraphanin or sulforaphane as the principal enzyme inducer) were highly effective in reducing the incidence, multiplicity, and rate of development of mammary tumors in dimethylbenz(a)anthracene-treated rats. Notably, sprouts of many broccoli cultivars contain negligible quantities of indole **glucosinolates**, which predominate in the mature vegetable and may give rise to degradation products (e.g., indole-3-carbinol) that can enhance tumorigenesis. Hence, small quantities of crucifer sprouts may protect against the risk of cancer as effectively as much larger quantities of mature vegetables of the same variety.

L11 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

ED Entered STN: 29 Nov 1996

ACCESSION NUMBER: 1996:708153 CAPLUS

DOCUMENT NUMBER: 126:6663

TITLE: Simultaneous Determination of
Isothiocyanates, Indoles, and
Oxazolidinethiones in **Myrosinase**
Digests of Rapeseeds and Rapeseed Meal by HPLC

AUTHOR(S): Matthaeus, B.; Fiebig, H.-J.

CORPORATE SOURCE: Institut fuer Chemie und Physik der Fette,
Bundesanstalt fuer Getreide- Kartoffel- und
Fettforschung, Muenster, D-48006, Germany

SOURCE: Journal of Agricultural and Food Chemistry
(1996), 44(12), 3894-3899

CODEN: JAFCAU; ISSN: 0021-8561

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB HPLC was used for the anal. of **isothiocyanates**, indoles, and oxazolidinethiones in rapeseeds and rapeseed meal. The samples were treated with **myrosinase** and the released hydrolysis products extracted with dichloromethane. The separation was performed on an RP-18 column using a gradient system with **acetonitrile** and water. Use of a programable UV detector permitted the detection of the compds. at their absorption maxima of 210 and 240 nm, resp. Response factors of eight standard compds. were calculated for 240 nm. The

contents of **glucosinolates** calculated with the results of this method showed a significant linear correlation ($r = 0.9995$; $P < 0.005$) with the contents of **glucosinolates** evaluated with the results of the HPLC method of desulfoglucosinolates.

IT 9025-38-1, **Myrosinase**

RL: ARU (Analytical role, unclassified); ANST (Analytical study)
(HPLC of degradation products in rapeseed **myrosinase** digests)

L11 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

ED Entered STN: 04 Oct 1992

ACCESSION NUMBER: 1992:530130 CAPLUS

DOCUMENT NUMBER: 117:130130

TITLE: Formation of indole **glucosinolates**
breakdown products during processing treatment
in Cruciferous vegetables

AUTHOR(S): Shim, Ki Hwan; Kang, Kap Suk; Sung, Nack Kie;
Seo, Kwon Il; Moon, Ju Seok

CORPORATE SOURCE: Dep. Food Sci. Technol., Gyeongsang Natl. Univ.,
Jinju, 660-701, S. Korea

SOURCE: Han'guk Yongyang Siklyong Hakhoechi (1992),
21(1), 49-53

CODEN: HYSHDL; ISSN: 0253-3154

DOCUMENT TYPE: Journal

LANGUAGE: Korean

AB The released amount of thiocyanate ion in Cruciferous vegetables treated by wet heat, increased with reaction time and was maximum after treatment for 30 min, but it was not changed by dry heat treatment. When samples were autolyzed by **myrosinase**, the amount of thiocyanate ion increased gradually with time was maximum after 3 h and much higher than those in the wet-treated in cabbage, decreasing in Chinese cabbage, radish, kale and mustard in that order. The generated amount of indoleacetonitrile by heat treatment increased with time and the generated amount in each sample determined was high in the order of cabbage, Chinese cabbage and radish.

IT 302-04-5, Thiocyanate, biological studies

RL: FORM (Formation, nonpreparative)
(formation of, from **glucosinolates** in cruciferous vegetable processing)

L11 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

ED Entered STN: 12 Jan 1991

ACCESSION NUMBER: 1991:6975 CAPLUS

DOCUMENT NUMBER: 114:6975

TITLE: Chemistry of indole **glucosinolates**:
intermediacy of indol-3-ylmethyl
isothiocyanates in the enzymic
hydrolysis of indole **glucosinolates**

AUTHOR(S): Hanley, A. Bryan; Parsley, Keith R.; Lewis,
Jenny A.; Fenwick, G. Roger

CORPORATE SOURCE: Inst. Food Res., AFRC, Norwich, NR4 7UA, UK

SOURCE: Journal of the Chemical Society, Perkin
Transactions 1: Organic and Bio-Organic
Chemistry (1972-1999) (1990), (8), 2273-6

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English
 OTHER SOURCE(S): CASREACT 114:6975
 AB The enzymic hydrolysis of 1-methoxyindol-3-ylmethyl **glucosinolate** proceeds via the corresponding **isothiocyanate**, thus providing evidence for a previously unsubstantiated breakdown pathway and establishing a link with 1-methoxycyclobrassinin and related indole phytoalexins.
 IT **9025-38-1, Myrosinase**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrolysis of indole **glucosinolates** by)

L11 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
 ED Entered STN: 25 Jun 1989
 ACCESSION NUMBER: 1989:230267 CAPLUS
 DOCUMENT NUMBER: 110:230267
 TITLE: Determination of **glucosinolates** in oilseed rape fodder by HPLC
 AUTHOR(S): Demes, H.; Marquard, R.; Zobelt, U.
 CORPORATE SOURCE: Inst. Pflanzenbau Pflanzenzuecht. I, Justus Liebig Univ., Giessen, D-6300, Fed. Rep. Ger.
 SOURCE: VDLUFA-Schriftenreihe (1989), 28(100 Jahre Agrarforsch. VA, Teil 2), 771-8
 CODEN: VDSCEE; ISSN: 0173-8712
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB **Glucosinolates** of rape forage were determined by drying (60°), grinding, extraction with hot MeOH, placing the sample on a Sephadex DEAE-25 column with an internal standard (sinigrin), washing with 0.2 M NaOAc buffer, desulfatation with sulfatase, elution with H2O, injection into a HPLC column (RP 18 ODS, 200 mm), elution with H2O-acetonitrile (80:20), and UV detection (229 nm). The drying of samples before grinding is emphasized, to eliminate **glucosinolate** degradation. Sampling methods are also discussed. Only small samples are necessary with this method, and **myrosinase** degradation is not needed. The **glucosinolate** contents of the rape green matter were not necessarily related to **glucosinolates** in the seeds.

L11 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
 ED Entered STN: 05 Apr 1987
 ACCESSION NUMBER: 1987:99205 CAPLUS
 DOCUMENT NUMBER: 106:99205
 TITLE: In vitro activity of **glucosinolates** and their products against *Leptosphaeria maculans*
 AUTHOR(S): Mithen, R. F.; Lewis, B. G.; Fenwick, G. R.
 CORPORATE SOURCE: Sch. Biol. Sci., Univ. East Anglia, Norwich, NR4 7TF, UK
 SOURCE: Transactions of the British Mycological Society (1986), 87(3), 433-40
 CODEN: BMSTA6; ISSN: 0007-1536
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The effects of a variety of **glucosinolates** and their hydrolysis products on the growth of *L. maculans* in culture were examined. When hydrolyzed with **myrosinase**, reaction products

of all the **glucosinolates** tested, except progoitrin (2-hydroxy-3-butenyl **glucosinolate**), were inhibitory; 2-propenyl **isothiocyanate**, derived from sinigrin, was the most toxic. Antifungal activity of indole hydrolysis products of glucobrassicin (3-indolylmethyl **glucosinolate**) and 1-methoxy glucobrassicin are described for the first time. Levels of **glucosinolates** reported to occur in leaves of oilseed rape correspond with levels shown here to be sufficient to generate strongly antifungal hydrolysis products. The significance of these compds. in resistance to *L. maculans* is discussed. In this context, the presence of indole **glucosinolate** in disproportionately high levels in low-**glucosinolate** cultivars of oilseed rape is of considerable interest.

L11 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

ED Entered STN: 12 May 1984

ACCESSION NUMBER: 1975:472939 CAPLUS

DOCUMENT NUMBER: 83:72939

TITLE: Aryl hydrocarbon hydroxylase induction in rat tissues by naturally occurring indoles of cruciferous plants

AUTHOR(S): Loub, William D.; Wattenberg, Lee W.; Davis, David W.

CORPORATE SOURCE: Dep. Lab. Med. Pathol., Univ. Minnesota, Minneapolis, MN, USA

SOURCE: Journal of the National Cancer Institute (1940-1978) (1975), 54(4), 985-8
CODEN: JNCIAM; ISSN: 0027-8874

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The aryl hydrocarbon hydroxylase [9037-52-9] inducers indole-3-**acetonitrile** (I) [771-51-7], indole-3-carbinol [700-06-1], and 3,3'-diindolylmethane [1968-05-4] were identified as naturally occurring in three cruciferous vegetables, Brussels sprouts, cabbage, and cauliflower. These compds. were produced during the hydrolysis of indolylmethyl **glucosinolate** [4356-52-9] by the plant enzyme **myrosinase** [9025-38-1].

IT 9025-38-1

RL: BIOL (Biological study)
(of crucifer, indolylmethyl **glucosinolate** hydrolysis by, aryl hydrocarbon hydroxylase inducer formation by)

(FILE 'MEDLINE, BIOSIS, EMBASE, WPIDS, CONFSCI, SCISEARCH, JICST-EPLUS, JAPIO, CABA, AGRICOLA, FSTA, LIFESCI, CANCERLIT'
ENTERED AT 12:14:49 ON 24 JUN 2004)

L12 7 S L8

L13 32 S L9

L14 7 S L10

L15 32 S L12 OR L13 OR L14

L16 16 DUP REM L15 (16 DUPLICATES REMOVED)

L16 ANSWER 1 OF 16 MEDLINE on STN

ACCESSION NUMBER: 2004070091 MEDLINE

DOCUMENT NUMBER: PubMed ID: 14871576

TITLE: In vitro digestion of sinigrin and glucotropaeolin by

single strains of Bifidobacterium and identification of the digestive products.

AUTHOR: Cheng D-L; Hashimoto K; Uda Y

CORPORATE SOURCE: Department of Bioproductive Sciences, Utsunomiya University, 350 Minemachi, Utsunomiya, 321-8505 Japan.

SOURCE: Food and chemical toxicology : an international journal published for the British Industrial Biological Research Association, (2004 Mar) 42 (3) 351-7.
Journal code: 8207483. ISSN: 0278-6915.

PUB. COUNTRY: England: United Kingdom

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200404

ENTRY DATE: Entered STN: 20040212
Last Updated on STN: 20040407
Entered Medline: 20040406

AB Three strains of Bifidobacterium sp., B. pseudocatenulatum, B. adolescentis, and B. longum were studied for their ability to digest **glucosinolates**, sinigrin (SNG) and glucotropaeolin (GTL), in vitro. All strains digested both **glucosinolates** during 24-48 h cultivation, accompanied by a decline in the medium pH from 7.1 to 5.2. The digestion of **glucosinolates** by a cell-free extract prepared from sonicated cells of B. adolescentis, but not cultivated broth, increased in the presence of 0.5 mM l-ascorbic acid. Also, a time-dependent formation of allyl **isothiocyanate** (AITC) was observed when the cell-free extract was incubated with 0.25 mM SNG for 120 min at pH 7.0. These reaction features suggest that the digestive activity may have been due to an enzyme similar to **myrosinase**, an enzyme of plant origin. GC-MS analysis of the Bifidobacterial cultured broth showed that the major products were 3-butenenitrile (BCN) and phenylacetonitrile (PhACN), from SNG and GTL, respectively and nitriles, probably due to a decrease in the pH of the media. AITC and benzyl **isothiocyanate** (BzITC) were barely detectable in the broth. It was concluded that the three species of Bifidobacteria could be involved in digestive degradation of **glucosinolates** in the human intestinal tract.

L16 ANSWER 2 OF 16 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN

ACCESSION NUMBER: 2003:509245 SCISEARCH

THE GENUINE ARTICLE: 687HU

TITLE: Separation and purification of **glucosinolates** from crude plant homogenates by high-speed counter-current chromatography

AUTHOR: Fahey J W (Reprint); Wade K L; Stephenson K K; Chou F E

CORPORATE SOURCE: Johns Hopkins Univ, Sch Med, Dept Pharmacol & Mol Sci, Lewis B & Dorothy Cullman Canc Chemoprotect Ctr, 406 WBSB, 725 N Wolfe St, Baltimore, MD 21205 USA (Reprint); Johns Hopkins Univ, Sch Med, Dept Pharmacol & Mol Sci, Lewis B & Dorothy Cullman Canc Chemoprotect Ctr, Baltimore, MD 21205 USA; Johns Hopkins Univ, Bloomberg Sch Publ Hlth, Ctr Human

Nutr, Baltimore, MD USA; Pharma Tech Res Corp,
Baltimore, MD 21212 USA
COUNTRY OF AUTHOR: USA
SOURCE: JOURNAL OF CHROMATOGRAPHY A, (9 MAY 2003) Vol. 996,
No. 1-2, pp. 85-93.
Publisher: ELSEVIER SCIENCE BV, PO BOX 211, 1000 AE
AMSTERDAM, NETHERLANDS.
ISSN: 0021-9673.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 26

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB **Glucosinolates** are anionic, hydrophilic plant secondary metabolites which are of particular interest due to their role in the prevention of cancer and other chronic and degenerative diseases. The separation and purification of **glucosinolates** from a variety of plant sources (e.g. seeds of broccoli, arugula and the horseradish tree), was achieved using high-speed counter-current chromatography (HSCCC). A high-salt, highly polar system containing 1-propanol-**acetonitrile**-saturated aqueous ammonium sulfate-water (1:0.5:1.2:1), was run on a semi-preparative scale and then transferred directly to preparative scale. Up to 7 g of a concentrated methanolic syrup containing about 10% **glucosinolates** was loaded on an 850-ml HSCCC column, and good separation and recovery were demonstrated for 4-methylsulfinylbutyl, 3-methyl-sulfinylpropyl, 4-methylthiobutyl, 2-propenyl and 4-(rhamnopyranosyloxy)benzyl **glucosinolates**. Multiple injections (5 to 6 times) were performed with well-preserved liquid stationary phase under centrifugal force. Pooled sequential runs with broccoli seed extract yielded about 20 g of its predominant **glucosinolate**, glucoraphanin, which was produced at >95% purity and reduced to powdered form. (C) 2003 Elsevier Science B.V. All rights reserved.

L16 ANSWER 3 OF 16 MEDLINE on STN DUPLICATE 1
ACCESSION NUMBER: 2001504897 MEDLINE
DOCUMENT NUMBER: PubMed ID: 11330806
TITLE: Direct determination of sinigrin in mustard seed without desulfatation by reversed-phase ion-pair liquid chromatography.
AUTHOR: Jen J F; Lin T H; Huang J W; Chung W C
CORPORATE SOURCE: Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan.. jfjen@mail.nchu.edu.tw
SOURCE: Journal of chromatography. A, (2001 Apr 6) 912 (2) 363-8.
Journal code: 9318488.
PUB. COUNTRY: Netherlands
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200109
ENTRY DATE: Entered STN: 20010917
Last Updated on STN: 20010917
Entered Medline: 20010913

AB Reversed-phase ion-pair liquid chromatography has been investigated for directly analyzing sinigrin in mustard seed without

desulfatation. After extraction by phosphate buffer (pH 7.0) from the grind-pastes of inactivated-**myrosinase** mustard seeds, sinigrin was first isolated through deproteinization and centrifugation, followed by filtration and injection into the chromatographic system. A reversed-phase C18 column was used to separate the sinigrin with an eluent of **acetonitrile** (ACN)-water (20:80) containing 0.02 M tetrabutylammonium (TBA) as the counter ion at pH 7.0. Detection was carried out with an UV detector operated at 227 nm. Factors affecting the chromatographic separation and quantitative determination, such as concentrations of TBA and ACN, and pH, were studied. The linear dynamic range is larger than three orders of magnitude and the detection limit is 0.045 mg/L. The RSD is around 3% and the recovery is 85% (3% RSD, n = 3).

L16 ANSWER 4 OF 16 CABA COPYRIGHT 2004 CABI on STN

ACCESSION NUMBER: 2002:9226 CABA

DOCUMENT NUMBER: 20013149702

TITLE: Hydrolysis products of **glucosinolates** from white cabbage (*Brassica oleracea* L.var Capitata) and cauliflower (*Brassica oleracea* L.var Botrytis) analyzed by HPLC and GC/MS

AUTHOR: Delonga, K.; Smit, Z.; Dragovic[acute]-Uzelac, V.; Mrkic[acute], V.; Vorkapic[acute]-Furac, J.; Pfannhauser, W. [EDITOR]; Fenwick, G. R. [EDITOR]; Khokhar, S. [EDITOR]

CORPORATE SOURCE: Faculty of Food Technology and Biotechnology, University of Zagreb, Pierottijeva 6, HR-10000 Zagreb, Croatia.

SOURCE: Biologically-active phytochemicals in food: analysis, metabolism, bioavailability and function. Proceedings of the EUROFOODCHEM XI Meeting, Norwich, UK, 26-28 September 2001, (2001) pp. 213-216. 5 ref.

Publisher: Royal Society of Chemistry. Cambridge

Price: Book chapter; Conference paper ; <pounds>69.50

Meeting Info.: Biologically-active phytochemicals in food: analysis, metabolism, bioavailability and function. Proceedings of the EUROFOODCHEM XI Meeting, Norwich, UK, 26-28 September 2001.

ISBN: 0-85404-806-5

PUB. COUNTRY: United Kingdom

DOCUMENT TYPE: Journal

LANGUAGE: English

ENTRY DATE: Entered STN: 20020111

Last Updated on STN: 20020111

AB In this study, the determination of **glucosinolates** (GSL) in cabbage and cauliflower, as well as their autolysis and hydrolysis products obtained by exogenous enzyme **myrosinase** was performed by reversed-phase high performance liquid chromatography (RP-LC) followed by gas-chromatography/mass spectrometry (GS/MS). The analysis data of the autolysis and hydrolysis products (pH 7.0) obtained by HPLC (DAD and FL detection)

and GC/MS confirmed that their relationship depends on GSL precursors and conditions of their enzymatic degradation (autolysis and hydrolysis). An examination of the indole GSL degradation products showed the presence of 4 to 7 different compounds. Three of them were identified as indole-3-carbinol (I3C), indole-3-acetonitrile (I3CN) and 3,3[prime]-diindolylmethane (DIM).

L16 ANSWER 5 OF 16 MEDLINE on STN
 ACCESSION NUMBER: 2000437676 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 10869674
 TITLE: Supercritical fluid chromatography as a method of analysis for the determination of 4-hydroxybenzylglucosinolate degradation products.
 AUTHOR: Buskov S; Hasselstrom J; Olsen C E; Sorensen H; Sorensen J C; Sorensen S
 CORPORATE SOURCE: Chemistry Department, Royal Veterinary and Agricultural University, Thorvaldsensvej 40, DK-1871, Frederiksberg C, Denmark.
 SOURCE: Journal of biochemical and biophysical methods, (2000 Jul 5) 43 (1-3) 157-74.
 Journal code: 7907378. ISSN: 0165-022X.
 PUB. COUNTRY: Netherlands
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 200009
 ENTRY DATE: Entered STN: 20000928
 Last Updated on STN: 20000928
 Entered Medline: 20000920

AB In the present study analytical and preparative supercritical fluid chromatography (SFC) were used for investigation of **myrosinase** catalysed degradation of 4-hydroxybenzylglucosinolate (sinalbin). Sinalbin occurs as a major **glucosinolate** in seeds of *Sinapis alba* L., in various mustards and other food products. The degradation products were identified and quantified by analysis based on a developed SFC method using a bare silica column. Determinations comprised transformation products of sinalbin, produced both during degradation of isolated sinalbin, and during autolysis of meal from *S. alba* seeds. The conditions in the developed SFC method were used as basis for the preparative SFC procedure applied for isolation of the components prior to their identification by nuclear magnetic resonance (NMR) spectroscopy. **Myrosinase** catalysed sinalbin hydrolysis resulted in the reactive 4-hydroxybenzyl **isothiocyanate** as an initial product at pH values from 3.5 to 7.5 whereas 4-hydroxybenzyl cyanide was one of the major products at low pH values. 4-Hydroxybenzyl **isothiocyanate** was found to disappear from the aqueous reaction mixtures in a few hours, as it reacted easily with available nucleophilic reagents. 4-Hydroxybenzyl alcohol was found as the product from reaction with water, and with ascorbic acid, 4-hydroxybenzylascorbigen was produced.

L16 ANSWER 6 OF 16 MEDLINE on STN DUPLICATE 2
 ACCESSION NUMBER: 97439871 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 9294217

TITLE: Broccoli sprouts: an exceptionally rich source of inducers of enzymes that protect against chemical carcinogens.

AUTHOR: Fahey J W; Zhang Y; Talalay P

CORPORATE SOURCE: Brassica Chemoprotection Laboratory and Department of Pharmacology and Molecular Sciences, The Johns Hopkins University School of Medicine, Baltimore, MD 21205, USA.

CONTRACT NUMBER: P01 CA 44530 (NCI)

SOURCE: Proceedings of the National Academy of Sciences of the United States of America, (1997 Sep 16) 94 (19) 10367-72.
Journal code: 7505876. ISSN: 0027-8424.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 199710

ENTRY DATE: Entered STN: 19971105
Last Updated on STN: 19971105
Entered Medline: 19971021

AB Induction of phase 2 detoxication enzymes [e.g., glutathione transferases, epoxide hydrolase, NAD(P)H: quinone reductase, and glucuronosyltransferases] is a powerful strategy for achieving protection against carcinogenesis, mutagenesis, and other forms of toxicity of electrophiles and reactive forms of oxygen. Since consumption of large quantities of fruit and vegetables is associated with a striking reduction in the risk of developing a variety of malignancies, it is of interest that a number of edible plants contain substantial quantities of compounds that regulate mammalian enzymes of xenobiotic metabolism. Thus, edible plants belonging to the family Cruciferae and genus Brassica (e.g., broccoli and cauliflower) contain substantial quantities of **isothiocyanates** (mostly in the form of their **glucosinolate** precursors) some of which (e.g., sulforaphane or 4-methylsulfinylbutyl **isothiocyanate**) are very potent inducers of phase 2 enzymes. Unexpectedly, 3-day-old sprouts of cultivars of certain crucifers including broccoli and cauliflower contain 10-100 times higher levels of glucoraphanin (the **glucosinolate** of sulforaphane) than do the corresponding mature plants. **Glucosinolates** and **isothiocyanates** can be efficiently extracted from plants, without hydrolysis of **glucosinolates** by **myrosinase**, by homogenization in a mixture of equal volumes of **dimethyl sulfoxide**, **dimethylformamide**, and **acetonitrile** at -50 degrees C. Extracts of 3-day-old broccoli sprouts (containing either glucoraphanin or sulforaphane as the principal enzyme inducer) were highly effective in reducing the incidence, multiplicity, and rate of development of mammary tumors in dimethylbenz(a)anthracene-treated rats. Notably, sprouts of many broccoli cultivars contain negligible quantities of indole **glucosinolates**, which predominate in the mature vegetable and may give rise to degradation products (e.g., indole-3-carbinol) that can enhance tumorigenesis. Hence, small quantities of crucifer sprouts may protect against the risk of cancer as effectively as much larger quantities of mature vegetables of the same variety.

L16 ANSWER 7 OF 16 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN
 DUPLICATE 3
 ACCESSION NUMBER: 97:882691 SCISEARCH
 THE GENUINE ARTICLE: YH162
 TITLE: Enzymatic, chemical, and thermal breakdown of
 H-3-labeled glucobrassicin, the parent indole
glucosinolate
 AUTHOR: Chevolleau S (Reprint); Gasc N; Rollin P; Tulliez J
 CORPORATE SOURCE: INRA, LAB XENOBIOT, BP 3, F-31931 TOULOUSE 9, FRANCE
 (Reprint); UNIV ORLEANS, ICOA, UPRESA 6005, F-45067
 ORLEANS 2, FRANCE
 COUNTRY OF AUTHOR: FRANCE
 SOURCE: JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY, (NOV
 1997) Vol. 45, No. 11, pp. 4290-4296.
 Publisher: AMER CHEMICAL SOC, 1155 16TH ST, NW,
 WASHINGTON, DC 20036.
 ISSN: 0021-8561.
 DOCUMENT TYPE: Article; Journal
 FILE SEGMENT: LIFE; AGRI
 LANGUAGE: English
 REFERENCE COUNT: 30

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The enzymatic, chemical, and thermal breakdown pathways of
 glucobrassicin, the major indolylmethyl **glucosinolate** of
 cruciferous vegetables, have been studied using synthetic
 H-3-labeled glucobrassicin (GBS). Radio-HPLC was used to analyze
 qualitatively and quantitatively the resulting products as well as
 their kinetics of formation. Enzymatic breakdown of GBS under
myrosinase action gave rise to different indole compounds
 [indole-3-carbinol (I3C), indole-3-**acetonitrile** (IAN) and
 3,3'-diindolylmethane (DIM)]. At neutral pH, GBS degradation was
 almost complete after 1 h, and the major breakdown product was I3C,
 which could be converted to DIM. The formation of this
 self-condensation product was observed as photosensitive. In acidic
 conditions, enzymatic degradation of GBS was a slower phenomenon,
 requiring 24 h to be nearly complete. IAN and I3C were the only two
 products occurring, and it was observed that the light had no effect
 either on the rate of formation or on the relative proportions of
 the breakdown products observed. GBS appeared as a very stable
 compound since no chemical degradation could be observed after 2 h
 in different aqueous media with pH in the 2-11 range. Moreover,
 after exposure to heat treatment, GBS was weakly degraded (10% in 1
 h), giving risk to a new minor indole condensation product
 corresponding to a 3-(indolylmethyl)glucobrassicin (IM-GBS).

L16 ANSWER 8 OF 16 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on
 STN DUPLICATE 4
 ACCESSION NUMBER: 1997:41907 BIOSIS
 DOCUMENT NUMBER: PREV199799333895
 TITLE: Simultaneous determination of **isothiocyanates**
 , indoles, and oxazolidinethiones in
myrosinase digests of rapeseeds and rapeseed
 meal by HPLC.
 AUTHOR(S): Matthaeus, B. [Reprint author]; Fiebig, H.-J.
 CORPORATE SOURCE: Institut fuer Chemie und Physik der Fette,

Bundesanstalt fuer Getreide- Kartoffel- und
Fettforschung, Postfach 1705, D-48006 Muenster,
Germany

SOURCE: Journal of Agricultural and Food Chemistry, (1996)
Vol. 44, No. 12, pp. 3894-3899.
CODEN: JAFCAU. ISSN: 0021-8561.

DOCUMENT TYPE: Article

LANGUAGE: English

ENTRY DATE: Entered STN: 28 Jan 1997
Last Updated on STN: 25 Mar 1997

AB HPLC has been used for the analysis of **isothiocyanates**,
indoles, and oxazolidinethiones in rapeseeds and rapeseed meal. The
samples were treated with **myrosinase** and the released
hydrolysis products extracted with dichloromethane. The separation
was performed on an RP-18 column using a gradient system with
acetonitrile and water. Use of a programmable UV detector
permitted the detection of the compounds at their absorption maxima
of 210 and 240 nm, respectively. Response factors of eight standard
compounds were calculated for 240 nm. The contents of
glucosinolates calculated with the results of this method
showed a significant linear correlation ($r = 0.9995$; $P \leq 0.005$)
with the contents of **glucosinolates** evaluated with the
results of the HPLC method of desulfoglucosinolates.

L16 ANSWER 9 OF 16 CABA COPYRIGHT 2004 CABI on STN

ACCESSION NUMBER: 92:146229 CABA

DOCUMENT NUMBER: 19921452451

TITLE: Formation of indole **glucosinolates**
breakdown products during processing treatment
in cruciferous vegetables

AUTHOR: Shim, K. H.; Kang, K. S.; Sung, N. K.; Seo, K.
I.; Moon, J. S.

CORPORATE SOURCE: Department of Food Science and Technology,
Gyeongsang National University, Jinju 660-701,
Korea Republic.

SOURCE: Journal of the Korean Society of Food and
Nutrition, (1992) Vol. 21, No. 1, pp. 49-53.
14 ref.
ISSN: 0253-3154

DOCUMENT TYPE: Journal

LANGUAGE: Korean

SUMMARY LANGUAGE: English

ENTRY DATE: Entered STN: 19941101
Last Updated on STN: 19941101

AB The released amount of thiocyanate ion in cruciferous vegetables
treated by wet heat, increased as a function of time and reached a
maximum value after 30 min, but did not change after dry heat
treatment. When samples were autolysed by **myrosinase**, the
amount of thiocyanate ion increased gradually, reached a maximum
value after 3 h and was higher than those treated by wet heat. The
released amount of thiocyanate ion in each sample was greatest in
cabbage, Chinese cabbage, radish, kale and mustard in that order.
The generated amount of indoleacetonitrile by heat treatment
increased as time elapsed, and the generated amount in each sample
was highest in cabbage, Chinese cabbage and radish, in that order.

L16 ANSWER 10 OF 16 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN
 ACCESSION NUMBER: 91:302382 SCISEARCH
 THE GENUINE ARTICLE: FM516
 TITLE: ROLE OF **GLUCOSINOLATES** IN THE FORMATION OF
 N-NITROSO COMPOUNDS
 AUTHOR: TIEDINK H G M (Reprint); MALINGRE C E; VANBROEKHOVEN
 L W; JONGEN W M F; LEWIS J; FENWICK G R
 CORPORATE SOURCE: AGR UNIV WAGENINGEN, DEPT TOXICOL, POB 8129, 6700 EV
 WAGENINGEN, NETHERLANDS (Reprint); CTR AGROBIOL RES,
 6700 AA WAGENINGEN, NETHERLANDS; AGROTECH RES INST,
 6700 AA WAGENINGEN, NETHERLANDS; AFRC, INST FOOD
 RES, NORWICH NR4 7UA, NORFOLK, ENGLAND
 COUNTRY OF AUTHOR: NETHERLANDS; ENGLAND
 SOURCE: JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY, (1991)
 Vol. 39, No. 5, pp. 922-926.
 DOCUMENT TYPE: Article; Journal
 FILE SEGMENT: LIFE; AGRI
 LANGUAGE: ENGLISH
 REFERENCE COUNT: 28

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The hydrolysis of the **glucosinolates**, sinigrin, gluconapin, glucobrassicinapin, progoitrin, glucotropaeolin, sinalbin, gluconasturtiin, glucobrassicin, and 4-hydroxyglucobrassicin, by **myrosinase** from white mustard (*Sinapis alba*) or acid was examined. While all **glucosinolates** were hydrolyzed by **myrosinase**, only 4-hydroxyglucobrassicin, glucosinalbin, gluconasturtiin, glucobrassicin, and progoitrin were partially hydrolyzed by acid (pH 2). When intact **glucosinolates** or **myrosinase**-treated **glucosinolate** products were treated with nitrite, only glucobrassicin and 4-hydroxyglucobrassicin formed N-nitroso compounds. The nitrosated products of **myrosinase**-treated glucobrassicin alone were mutagenic and induced about 400 *Salmonella typhimurium* TA100 revertants/ μ -mol. The enzymic breakdown products of the alkyl and aryl **glucosinolates** were cytotoxic, but this activity was not affected by subsequent nitrite treatment. Given the levels at which indole **glucosinolates** occur in brassica vegetables, these findings suggest that their contribution to the observed mutagenic potential of these vegetables after nitrite treatment will be marginal. Further work is, however, needed to identify the exact chemical natures of both the N-nitroso compounds formed in nitrite-treated brassicas and their naturally occurring precursors.

L16 ANSWER 11 OF 16 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 1984:342461 BIOSIS
 DOCUMENT NUMBER: PREV198478078941; BA78:78941
 TITLE: PRELIMINARY STUDIES ON THE EFFECTS OF COPPER IRON AND MANGANESE IONS ON THE DEGRADATION OF 3 INDOLYLMETHYL **GLUCOSINOLATE** A CONSTITUENT OF BRASSICA-SPP BY **MYROSINASE** EC-3.2.3.1.
 AUTHOR(S): SEARLE L M [Reprint author]; CHAMBERLAIN K; BUTCHER D N
 CORPORATE SOURCE: ROTHAMSTED EXPERIMENTAL STATION, HARPENDEN, HERTS AL5 2JQ, UK

09/825989

SOURCE: Journal of the Science of Food and Agriculture,
(1984) Vol. 35, No. 7, pp. 745-748.
CODEN: JSFAAE. ISSN: 0022-5142.

DOCUMENT TYPE: Article

FILE SEGMENT: BA

LANGUAGE: ENGLISH

AB Cu (I and II) and Fe (II and III) ions had qualitatively similar effects on the degradation of radiolabeled 3-indolylmethylglucosinolate. In the presence of **myrosinase** they increased the production of 3-indolylacetonitrile (IAN) largely at the expense of ascorbigen (ASC). With the addition of these metal ions the ratio of IAN to the products of the alternative pathways (3,3'-diindolylmethane, ASC and formaldehyde) decreased as the pH increased from 4 to 7. These ions also led to a small increase in the non-enzymic production of IAN.

L16 ANSWER 12 OF 16 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1983:233173 BIOSIS

DOCUMENT NUMBER: PREV198375083173; BA75:83173

TITLE: THE CONVERSION OF 3 INDOLYLMETHYL
GLUCOSINOLATE TO 3 INDOLYL
ACETONITRILE BY **MYROSINASE** AND ITS
RELEVANCE TO THE CLUBROOT DISEASE OF THE CRUCIFERAE.

AUTHOR(S): SEARLE L M [Reprint author]; CHAMBERLAIN K; RAUSCH T;
BUTCHER D N

CORPORATE SOURCE: ROTHAMSTED EXPERIMENTAL STATION, HARPENDEN, HERTS AL5
2JQ, UK

SOURCE: Journal of Experimental Botany, (1982) Vol. 33, No.
136, pp. 935-942.
CODEN: JEBOA6. ISSN: 0022-0957.

DOCUMENT TYPE: Article

FILE SEGMENT: BA

LANGUAGE: ENGLISH

AB [Methylene-14C]-3-indolylmethylglucosinolate (14C-IMG) was converted in vitro to [methylene-14C]-3-indolylacetonitrile (14C-IAN) by **myrosinase** [thioglucoside glucohydrolase EC 3.2.3.1] over a pH range of 4.0-6.0 and this conversion was enhanced by ferrous ions. Other products of the reaction included 3-indolylmethanol, 3,3'-diindolylmethane and ascorbigen A. Trace amounts of 14C-IAN were produced non-enzymically from 14C-IMG in the presence of ferrous ion over a similar pH range. Furthermore, swede tissues (Brassica napus cv. Danestone) infected with Plasmodiophora brassicae Woron. could convert 14C-IMG to 14C-IAN. These results were consistent with the hypothesis that the overgrowth symptoms of the clubroot disease are caused by the conversion of IMG to the auxin precursor IAN.

L16 ANSWER 13 OF 16 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
DUPLICATE 5

ACCESSION NUMBER: 1980:200330 BIOSIS

DOCUMENT NUMBER: PREV198069075326; BA69:75326

TITLE: AN HIGH PRESSURE LIQUID CHROMATOGRAPHIC METHOD FOR
SIMULTANEOUS QUANTITATION OF INDIVIDUAL **ISO**
THIO CYANATES AND OXAZOLIDINETHIONE
IN **MYROSINASE** EC-3.2.3.1 DIGESTS OF

Searcher : Shears 571-272-2528

RAPESEED MEAL.
 AUTHOR(S): MAHESHWARI P N [Reprint author]; STANLEY D W; GRAY J I; VOORT F R
 CORPORATE SOURCE: DEP FOOD SCI, UNIV GUELPH, GUELPH, ONT N1G 2W1, CAN
 SOURCE: Journal of the American Oil Chemists' Society, (1979)
 Vol. 56, No. 9, pp. 837-841.
 CODEN: JAOCA7. ISSN: 0003-021X.
 DOCUMENT TYPE: Article
 FILE SEGMENT: BA
 LANGUAGE: ENGLISH

AB A simple, rapid and precise method for simultaneous quantitation of individual **isothiocyanates** and oxazolidinethione in **myrosinase** digests of rapeseed meal has been developed. The method consists of inactivation of native **myrosinase** activity present in the seedmeal, followed by digestion with mustard **myrosinase** (thioglucoside glucohydrolase, EC 3.2.3.1) to hydrolyze rapeseed **glucosinolates** quantitatively to **isothiocyanates** and oxazolidinethione. These hydrolytic products are extracted in methylene chloride as soon as they are formed and finally resolved by a reverse phase high pressure liquid chromatography (HPLC) technique on a μ Bondapak C18 column using aqueous **acetonitrile** as solvent and an UV absorbance detector set at 254 nm. The lower limits of quantitation by this method in a single aliquot applied to the column were 0.2 μ g for the **isothiocyanates** and 0.01 μ g for the oxazolidinethione. Recoveries of allyl **isothiocyanate**, oxazolidinethione and sinigrin added to Brassica juncea, prior to digestion, were quantitative and averaged at 94.5, 93.0 and 91.2% with SD of 1.5, 3.3 and 2.8%, respectively. The butenyl and pentenyl **isothiocyanates** and oxazolidinethione in Tower (B. napus) and Candle (B. campestris) rapeseeds, and allyl **isothiocyanate** in B. juncea were the major hydrolytic products of **glucosinolates**. The identity of peaks corresponding to these compounds on a HPLC chromatogram was confirmed by mass spectroscopy.

L16 ANSWER 14 OF 16 MEDLINE on STN DUPLICATE 6
 ACCESSION NUMBER: 75153618 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 1127728
 TITLE: Aryl hydrocarbon hydroxylase induction in rat tissues by naturally occurring indoles of cruciferous plants.
 AUTHOR: Loub W D; Wattenberg L W; Davis D W
 SOURCE: Journal of the National Cancer Institute, (1975 Apr) 54 (4) 985-8.
 Journal code: 7503089. ISSN: 0027-8874.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 197507
 ENTRY DATE: Entered STN: 19900310
 Last Updated on STN: 19970203
 Entered Medline: 19750724

AB A phytochemical investigation to identify inducers of increased aryl hydrocarbon hydroxylase (AHH) activity from three cruciferous vegetables, Brussels sprouts, cabbage, and cauliflower, resulted in

the identification of indole-3-**acetonitrile**, indole-3-carbinol, and 3,3'-diindolylmethane as naturally occurring inducers. These compounds are produced during the hydrolysis of indolyl-methyl **glucosinolate** by the plant enzyme **myrosinase**.

L16 ANSWER 15 OF 16 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1974:169038 BIOSIS
DOCUMENT NUMBER: PREV197457068738; BA57:68738
TITLE: THE ROLE OF INDOLE **GLUCOSINOLATES** IN THE CLUB ROOT DISEASE OF THE CRUCIFERAE.
AUTHOR(S): BUTCHER D N; EL-TIGANI S; INGRAM D S
SOURCE: Physiological Plant Pathology, (1974) Vol. 4, No. 1, pp. 127-140.
CODEN: PPPYBC. ISSN: 0048-4059.
DOCUMENT TYPE: Article
FILE SEGMENT: BA
LANGUAGE: Unavailable

L16 ANSWER 16 OF 16 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1970:205651 BIOSIS
DOCUMENT NUMBER: PREV197051115651; BA51:115651
TITLE: INDOLE **ACETO NITRILE** SYNTHESIS FROM GLUCOBRASSICIN PH DEPENDENCE AND IMPORTANCE FOR GROWTH.
AUTHOR(S): SCHRAUDOLF H; WEBER H
SOURCE: Planta (Heidelberg), (1969) Vol. 88, No. 2, pp. 136-143.
CODEN: PLANAB. ISSN: 0032-0935.
DOCUMENT TYPE: Article
FILE SEGMENT: BA
LANGUAGE: Unavailable

FILE 'CAPLUS' ENTERED AT 12:16:48 ON 24 JUN 2004

L17 1 S L4 AND (DMSO OR DMF)
L18 0 S L17 NOT L11

FILE 'MEDLINE, BIOSIS, EMBASE, WPIDS, CONFSCI, SCISEARCH, JICST-EPLUS, JAPIO, CABA, AGRICOLA, FSTA, LIFESCI, CANCERLIT' ENTERED AT 12:17:15 ON 24 JUN 2004

L19 1 S L17
L20 1 S L19 NOT L15

L20 ANSWER 1 OF 1 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 2003:513019 BIOSIS
DOCUMENT NUMBER: PREV200300516359
TITLE: A facile and efficient synthesis of 14C-labelled sulforaphane.
AUTHOR(S): D'Souza, Christopher A.; Amin, Shantu; Desai, Dhimant [Reprint Author]
CORPORATE SOURCE: Institute for Cancer Prevention, 1 Dana Road, Valhalla, NY, 10595, USA
ddesai@ifcp.us

09/825989

SOURCE: Journal of Labelled Compounds and
Radiopharmaceuticals, (August 2003) Vol. 46, No. 9,
pp. 851-859. print.
ISSN: 0362-4803 (ISSN print).

DOCUMENT TYPE: Article

LANGUAGE: English

ENTRY DATE: Entered STN: 5 Nov 2003

Last Updated on STN: 5 Nov 2003

AB **Isothiocyanates** have gained considerable attention for their role as potent chemopreventive agents. Sulforaphane, 1a (SFN), a naturally occurring **isothiocyanate**, was isotopically labelled in five steps starting from 3-(methylthio)-1-propanol (2). Reacting 2 with tosyl chloride in the presence of Et₃N yielded the tosylate 3. Gently refluxing 3 with K¹⁴CN in DMF gave the nitrile 4b. Reduction to the amine 5b was achieved using BH₃-THF. Oxidation with 30% hydrogen peroxide followed by treatment with thiophosgene yielded (+-)(1-¹⁴C)SFN, 1b. The overall radiochemical yield was 4.4% based on the starting K¹⁴CN.

(FILE 'CAPLUS' ENTERED AT 12:18:20 ON 24 JUN 2004)

L1 1 SEA FILE=REGISTRY ABB=ON PLU=ON ISOTHIOCYANATE/CN
L3 32844 SEA FILE=CAPLUS ABB=ON PLU=ON L1 OR ISOTHIOCYANATE OR
ISO(W) (THIOCYANATE OR THIO CYANATE) OR ISOTHIO CYANATE
OR GLUCOSINOLATE
L5 1 SEA FILE=REGISTRY ABB=ON PLU=ON "DIMETHYL SULFOXIDE"/CN
L6 2 SEA FILE=REGISTRY ABB=ON PLU=ON (ACETONITRILE/CN OR
"ACETONITRILE (13CH3CN)"/CN)
L7 1 SEA FILE=REGISTRY ABB=ON PLU=ON DIMETHYLFORMAMIDE/CN
L21 56709 SEA FILE=CAPLUS ABB=ON PLU=ON (L5 OR DIMETHYLSULFOXIDE
OR DIMETHYLSULPHOXIDE OR DI(W) (METHYLSULFOXIDE OR
METHYLSULPHOXIDE OR (ME OR METHYL) (W) (SULFOXIDE OR
SULPHOXIDE)) OR DIMETHYL(W) (SULFOXIDE OR SULPHOXIDE) OR
DMSO)
L22 4851 SEA FILE=CAPLUS ABB=ON PLU=ON L21 AND (L6 OR ACETONITRI
LE OR ACETO NITRILE)
L23 2784 SEA FILE=CAPLUS ABB=ON PLU=ON L22 AND (L7 OR DIMETHYLFO
RMAMIDE OR DI(W) (METHYLFORMAMIDE OR (ME OR METHYL) (W) FORM
AMIDE) OR DIMETHYL FORMAMIDE OR DMF)
L24 34 SEA FILE=CAPLUS ABB=ON PLU=ON L23 AND L3
L25 2 SEA FILE=CAPLUS ABB=ON PLU=ON L24 AND (EXTRACT? OR
EXT##)

L26 1 L25 NOT L11

L26 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

ED Entered STN: 12 May 1984

ACCESSION NUMBER: 1981:128527 CAPLUS

DOCUMENT NUMBER: 94:128527

TITLE: Anion solvation free energies from distribution
equilibriums

AUTHOR(S): Marcus, Y.; Pross, E.; Hormadaly, J.

CORPORATE SOURCE: Dep. Inorg. Anal. Chem., Hebrew Univ.,
Jerusalem, Israel

Searcher : Shears 571-272-2528

SOURCE: Int. Solvent Extr. Conf., [Proc.] (1980), Volume
3, Paper 80-117, 8 pp.. Assoc. Ing. Univ.
Liege: Liege, Belg.
CODEN: 45DZA9

DOCUMENT TYPE: Conference

LANGUAGE: English

AB The solvation Gibbs free energies of anions (X-) are key items for understanding the solvent **extraction** equilibrium Transfer Gibbs free energies, $\Delta G_t^\circ(X-, W \rightarrow S)$, based on the tetraphenylarsonium tetraphenylborate [15627-12-0] assumption, represent them adequately. Data for these for 11 anions X- and 15 solvents S are tabulated, and expressed parametrically as $\Delta G_t^\circ(X-, W \rightarrow S) = a(X-) + b(X-)[ET(W) - ET(S)]$ in terms of the solvent polarity index ET. A distribution method, based on the sequestration of K⁺ by crown ethers, provides exptl. data for anion transfer between water and immiscible solvents, relevant to solvent **extraction**. The equation used is $\Delta G_t^\circ(X-, W \rightarrow S) = -RT \ln K_{\text{distr}}(X-, S/W) + p(1/\epsilon_S) + q$, where K is the equilibrium constant for the ion-pair **extraction** of KCw+X (Cw is the crown ether), ϵ_S the dielec. constant, p an independently known constant, and q must be obtained by calibration with a solvent with known $\Delta G_t^\circ(X-, W \rightarrow S)$.

IT 67-68-5, properties 68-12-2, properties

75-05-8, properties

RL: PRP (Properties)

(free energy of transfer and anions from water to)

IT 302-04-5, properties

RL: PRP (Properties)

(free energy of transfer of, from water to solvent, solvation in relation to)

(FILE 'MEDLINE, BIOSIS, EMBASE, WPIDS, CONFSCI, SCISEARCH, JICST-EPLUS, JAPIO, CABA, AGRICOLA, FSTA, LIFESCI, CANCERLIT' ENTERED AT 12:22:16 ON 24 JUN 2004)

L27 8 S L25

L28 1 S L27 NOT (L15 OR L19)

L28 ANSWER 1 OF 1 EMBASE COPYRIGHT 2004 ELSEVIER INC. ALL RIGHTS RESERVED. on STN

ACCESSION NUMBER: 1998153219 EMBASE

TITLE: Solvent **extraction** of europium from aqueous-organic solutions by solvating **extractants**.

AUTHOR: Hala J.

CORPORATE SOURCE: J. Hala, Department of Inorganic Chemistry, Masaryk University, Kotlarska 2, 61137 Brno, Czech Republic

SOURCE: Journal of Radioanalytical and Nuclear Chemistry, (1998) 230/1-2 (135-141).

Refs: 21

ISSN: 0236-5731 CODEN: JRNCMD

COUNTRY: Hungary

DOCUMENT TYPE: Journal; Article

FILE SEGMENT: 029 Clinical Biochemistry

LANGUAGE: English

SUMMARY LANGUAGE: English

AB The partition of Eu(III) between benzene containing solvating **extractants** (TBP, TOPO, dioctylsulfoxide) and aqueous nitrate, perchlorate and thiocyanate solutions containing various organic solvents miscible with water (alcohols, acetone, **acetonitrile**, ethylene glycol, **dimethyl sulfoxide** and **dimethylformamide**) was investigated. Depending on the specific **extraction** system, the presence of organic solvents in the mixed phase showed various effects on the distribution ratio of Eu(III). These were discussed in terms of solute-solvent interactions. The results in the systems containing **dimethylformamide** and **dimethyl sulfoxide** indicated complexation of Eu(III) with these solvents in the polar phase.

FILE 'CAPLUS' ENTERED AT 12:27:04 ON 24 JUN 2004

L31 8 SEA ABB=ON PLU=ON L3 AND (THIOGLYCOSIDASE OR THIO
GLYCOSIDASE OR GLUCOSINOLASE)
L32 0 SEA ABB=ON PLU=ON L31 AND (L5 OR DIMETHYLSULFOXIDE OR
DIMETHYLSULPHOXIDE OR DI(W) (METHYLSULFOXIDE OR METHYLSULP
HOXIDE OR (ME OR METHYL) (W) (SULFOXIDE OR SULPHOXIDE)) OR
DIMETHYL(W) (SULFOXIDE OR SULPHOXIDE) OR DMSO)
L33 0 SEA ABB=ON PLU=ON L31 AND (L6 OR ACETONITRILE OR ACETO
NITRILE)
L34 0 SEA ABB=ON PLU=ON L31 AND (L7 OR DIMETHYLFORMAMIDE OR
DI(W) (METHYLFORMAMIDE OR (ME OR METHYL) (W) FORMAMIDE) OR
DIMETHYL FORMAMIDE OR DMF)

FILE 'MEDLINE, BIOSIS, EMBASE, WPIDS, CONFSCI, SCISEARCH,
JICST-EPLUS, JAPIO, CABA, AGRICOLA, FSTA, LIFESCI, CANCERLIT'
ENTERED AT 12:28:24 ON 24 JUN 2004

L35 0 SEA ABB=ON PLU=ON L32
L36 1 SEA ABB=ON PLU=ON L33
L37 0 SEA ABB=ON PLU=ON L34
L38 0 SEA ABB=ON PLU=ON L36 NOT (L15 OR L19 OR L28)

(FILE 'MEDLINE' ENTERED AT 12:30:40 ON 24 JUN 2004)

L29 872 SEA FILE=MEDLINE ABB=ON PLU=ON ISOTHIOCYANATES/CT
L30 329 SEA FILE=MEDLINE ABB=ON PLU=ON GLUCOSINOLATES/CT
L43 1265 SEA FILE=MEDLINE ABB=ON PLU=ON ACETONITRILES/CT
L44 1061 SEA FILE=MEDLINE ABB=ON PLU=ON DIMETHYLFORMAMIDE/CT
L45 9846 SEA FILE=MEDLINE ABB=ON PLU=ON "DIMETHYL SULFOXIDE"/CT
L47 8 SEA FILE=MEDLINE ABB=ON PLU=ON (L29 OR L30) AND (L43
OR L44 OR L45)

L47 ANSWER 1 OF 8 MEDLINE on STN
ACCESSION NUMBER: 2004070091 MEDLINE
DOCUMENT NUMBER: PubMed ID: 14871576
TITLE: In vitro digestion of sinigrin and glucotropaeolin by
single strains of Bifidobacterium and identification
of the digestive products.
AUTHOR: Cheng D-L; Hashimoto K; Uda Y
CORPORATE SOURCE: Department of Bioproductive Sciences, Utsunomiya
University, 350 Minemachi, Utsunomiya, 321-8505
Japan.
SOURCE: Food and chemical toxicology : an international

09/825989

journal published for the British Industrial
Biological Research Association, (2004 Mar) 42 (3)
351-7.

Journal code: 8207483. ISSN: 0278-6915.

PUB. COUNTRY: England: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200404
ENTRY DATE: Entered STN: 20040212
Last Updated on STN: 20040407
Entered Medline: 20040406

ED Entered STN: 20040212
Last Updated on STN: 20040407
Entered Medline: 20040406

AB Three strains of *Bifidobacterium* sp., *B. pseudocatenulatum*, *B. adolescentis*, and *B. longum* were studied for their ability to digest glucosinolates, sinigrin (SNG) and glucotropaeolin (GTL), in vitro. All strains digested both glucosinolates during 24-48 h cultivation, accompanied by a decline in the medium pH from 7.1 to 5.2. The digestion of glucosinolates by a cell-free extract prepared from sonicated cells of *B. adolescentis*, but not cultivated broth, increased in the presence of 0.5 mM l-ascorbic acid. Also, a time-dependent formation of allyl isothiocyanate (AITC) was observed when the cell-free extract was incubated with 0.25 mM SNG for 120 min at pH 7.0. These reaction features suggest that the digestive activity may have been due to an enzyme similar to myrosinase, an enzyme of plant origin. GC-MS analysis of the *Bifidobacterium* cultured broth showed that the major products were 3-butenenitrile (BCN) and phenylacetonitrile (PhACN), from SNG and GTL, respectively and nitriles, probably due to a decrease in the pH of the media. AITC and benzyl isothiocyanate (BzITC) were barely detectable in the broth. It was concluded that the three species of *Bifidobacteria* could be involved in digestive degradation of glucosinolates in the human intestinal tract.

L47 ANSWER 2 OF 8 MEDLINE on STN
ACCESSION NUMBER: 2000437676 MEDLINE
DOCUMENT NUMBER: PubMed ID: 10869674
TITLE: Supercritical fluid chromatography as a method of
analysis for the determination of
4-hydroxybenzylglucosinolate degradation products.
AUTHOR: Buskov S; Hasselstrom J; Olsen C E; Sorensen H;
Sorensen J C; Sorensen S
CORPORATE SOURCE: Chemistry Department, Royal Veterinary and
Agricultural University, Thorvaldsensvej 40, DK-1871,
Frederiksberg C, Denmark.
SOURCE: Journal of biochemical and biophysical methods, (2000
Jul 5) 43 (1-3) 157-74.
Journal code: 7907378. ISSN: 0165-022X.
PUB. COUNTRY: Netherlands
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200009
ENTRY DATE: Entered STN: 20000928

Searcher : Shears 571-272-2528

Last Updated on STN: 20000928

Entered Medline: 20000920

ED Entered STN: 20000928

Last Updated on STN: 20000928

Entered Medline: 20000920

AB In the present study analytical and preparative supercritical fluid chromatography (SFC) were used for investigation of myrosinase catalysed degradation of 4-hydroxybenzylglucosinolate (sinalbin). Sinalbin occurs as a major glucosinolate in seeds of *Sinapis alba* L., in various mustards and other food products. The degradation products were identified and quantified by analysis based on a developed SFC method using a bare silica column. Determinations comprised transformation products of sinalbin, produced both during degradation of isolated sinalbin, and during autolysis of meal from *S. alba* seeds. The conditions in the developed SFC method were used as basis for the preparative SFC procedure applied for isolation of the components prior to their identification by nuclear magnetic resonance (NMR) spectroscopy. Myrosinase catalysed sinalbin hydrolysis resulted in the reactive 4-hydroxybenzyl isothiocyanate as an initial product at pH values from 3.5 to 7.5 whereas 4-hydroxybenzyl cyanide was one of the major products at low pH values. 4-Hydroxybenzyl isothiocyanate was found to disappear from the aqueous reaction mixtures in a few hours, as it reacted easily with available nucleophilic reagents. 4-Hydroxybenzyl alcohol was found as the product from reaction with water, and with ascorbic acid, 4-hydroxybenzylascorbigen was produced.

L47 ANSWER 3 OF 8

MEDLINE on STN

ACCESSION NUMBER: 2000244162 MEDLINE

DOCUMENT NUMBER: PubMed ID: 10782305

TITLE: Synthesis of 6,7-dideoxy-7-isothiocyanatoheptoses: stable fully unprotected monosaccharide isothiocyanates.

AUTHOR: Benito J M; Oriz Mellet C; Garcia Fernandez J M

CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Quimica, Universidad de Sevilla, Spain.

SOURCE: Carbohydrate research, (2000 Jan 12) 323 (1-4) 218-25.

Journal code: 0043535. ISSN: 0008-6215.

PUB. COUNTRY: Netherlands

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200007

ENTRY DATE: Entered STN: 20000720

Last Updated on STN: 20000720

Entered Medline: 20000710

ED Entered STN: 20000720

Last Updated on STN: 20000720

Entered Medline: 20000710

AB Methyl 6,7-dideoxy-7-isothiocyanato-alpha-D-gluco (manno) (galacto)-heptopyranosides have been synthesized in four steps by homologation of the respective methyl hexopyranosides via the corresponding heptopyranosyduronitriles. Neither intra- nor intermolecular thiocarbamate formation was observed, even under rather strenuous acidic or basic conditions. The reducing

derivative 6,7-dideoxy-7-isothiocyanato-alpha-D-glucopyranose was also a stable compound in aqueous solution in the absence of base. Formation of a six-membered intramolecular cyclic thiocarbamate was achieved in DMF solution in the presence of triethylamine. The title compounds are the first examples of stable fully unprotected monosaccharide isothiocyanates.

L47 ANSWER 4 OF 8 MEDLINE on STN
 ACCESSION NUMBER: 96193067 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 8610048
 TITLE: Selective toxicity of compounds naturally present in food toward the transformed phenotype of human colorectal cell line HT29.
 AUTHOR: Musk S R; Stephenson P; Smith T K; Stening P; Fyfe D; Johnson I T
 CORPORATE SOURCE: Agricultural and Food Research Council, institute of Food Research, Norwich Laboratory, UK.
 SOURCE: Nutrition and cancer, (1995) 24 (3) 289-98.
 Journal code: 7905040. ISSN: 0163-5581.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199605
 ENTRY DATE: Entered STN: 19960605
 Last Updated on STN: 19990129
 Entered Medline: 19960524

ED Entered STN: 19960605
 Last Updated on STN: 19990129
 Entered Medline: 19960524

AB It has previously been observed that allyl isothiocyanate, a compound naturally present in the diet, is more cytotoxic toward the human colorectal adenocarcinoma cell line HT29 in its control transformed state than after exposure to sodium butyrate or to dimethylformamide, which slow growth and induce differentiation (detransformation). In the present study, a range of other dietary compounds were assayed for such selective toxicity. These compounds were chosen as constituents of foodstuffs that have been identified from epidemiologic studies as being potentially antitumorigenic and also as having anticarcinogenic activity in experimental models. Benzyl and phenethyl isothiocyanate, benzyl thiocyanate, and quercetin showed decreased toxicity towards HT29 after detransformation of the cells by one or both treatments, whereas no change was observed in the sensitivity to diallyl sulfide or diallyl disulfide. It is proposed that the presence of such selectively toxic compounds in the diet may inhibit the development of tumors by interfering with the growth of preneoplastic lesions while having little effect on normal cells. The cumulative effects of these inhibitions may contribute to the chemopreventive properties of the parent foodstuffs observed in epidemiologic studies.

L47 ANSWER 5 OF 8 MEDLINE on STN
 ACCESSION NUMBER: 94037293 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 8222057
 TITLE: Allyl isothiocyanate is selectively toxic to transformed cells of the human colorectal tumour line

HT29.
 AUTHOR: Musk S R; Johnson I T
 CORPORATE SOURCE: AFRC Institute of Food Research, Norwich Laboratory,
 Norwich Research Park, Colney, Norfolk, UK.
 SOURCE: Carcinogenesis, (1993 Oct) 14 (10) 2079-83.
 Journal code: 8008055. ISSN: 0143-3334.
 PUB. COUNTRY: ENGLAND: United Kingdom
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199312
 ENTRY DATE: Entered STN: 19940117
 Last Updated on STN: 19990129
 Entered Medline: 19931201

ED Entered STN: 19940117
 Last Updated on STN: 19990129
 Entered Medline: 19931201

AB Allyl isothiocyanate, a constituent of mustard and certain vegetables found in the human diet, was tested for cytotoxic and cytostatic effects in HT29 human colon carcinoma cells in vitro. For an exposure time of 24 h, allyl isothiocyanate exhibited a Dq of 0.32 microgram/ml and a D0 of 0.74 micrograms/ml. Following detransformation of the cells by treatment with sodium butyrate or dimethylformamide the cells became more resistant to the cytotoxic effects of allyl isothiocyanate, the Dq increasing to 0.74 microgram/ml and the D0 to 0.96 microgram/ml (with butyrate) or 0.84 microgram/ml (with dimethylformamide). At the Dq value for detransformed cells the survival of the control cells was reduced to 56%. Allyl isothiocyanate was also found to be less cytostatic to the mass growth of detransformed populations in that daily doses of 1.6 micrograms/ml over a week reduced the final number of detransformed cells relative to untreated cultures by < 25% whilst growth of the transformed cultures was reduced by > 60%. Given this increased sensitivity of the cells to allyl isothiocyanate when in the transformed state, it is hypothesized that, when consumed in the human diet, this compound may protect against the development of colorectal cancer by selectively inhibiting the growth of transformed cell clones within the gastrointestinal mucosa.

L47 ANSWER 6 OF 8 MEDLINE on STN
 ACCESSION NUMBER: 92098517 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 1757417
 TITLE: A new approach to the study of glucosinolates by isocratic liquid chromatography. Part I. Rapid determination of desulfated derivatives of rapeseed glucosinolates.
 AUTHOR: Quinsac A; Ribaillier D; Elfakir C; Lafosse M; Dreux M
 CORPORATE SOURCE: Centre Technique Interprofessionnel des Oleagineux Metropolitains, Ardon, France.
 SOURCE: Journal - Association of Official Analytical Chemists, (1991 Nov-Dec) 74 (6) 932-9.
 Journal code: 7505559. ISSN: 0004-5756.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English

FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199202
 ENTRY DATE: Entered STN: 19920223
 Last Updated on STN: 19980206
 Entered Medline: 19920206

ED Entered STN: 19920223
 Last Updated on STN: 19980206
 Entered Medline: 19920206

AB Liquid chromatographic (LC) analysis of desulfated derivatives of rapeseed glucosinolates has been carried out under isocratic elution conditions with different CN-bonded stationary phases. The effects of the eluant composition (water, acetonitrile, and methanol) with the stationary phase (Zorbax CN, Lichrospher CN, and Ultrasphere CN) and temperature (20 and 50 degrees C) are described. An isocratic LC method performed at room temperature using a Lichrospher CN column and water as mobile phase is proposed. The chromatographic analysis can be done in less than 12 min, and it is easier and less expensive than the traditional gradient mode. Four commercial samples of rapeseed containing various quantities of other cruciferous seeds (wild mustard and stinkweed) as an admixture have been analyzed to determine the total glucosinolate content. Relative standard deviations of repeatability of the isocratic and gradient LC methods ranged from 0.4 to 1.7% and from 2.7 to 4.7%, respectively. Comparison of the results showed good agreement between the 2 methods (better than 98%).

L47 ANSWER 7 OF 8 MEDLINE on STN
 ACCESSION NUMBER: 88272993 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 3391960
 TITLE: Characterization of benzyl isothiocyanate and phenyl acetonitrile from papayas by mass spectrometry.
 AUTHOR: Cairns T; Siegmund E G; Stamp J J; Jacobs R M
 CORPORATE SOURCE: Food and Drug Administration, Office of Regulatory Affairs, Los Angeles, CA 90015.
 SOURCE: Journal - Association of Official Analytical Chemists, (1988 May-Jun) 71 (3) 547-50.
 Journal code: 7505559. ISSN: 0004-5756.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 198808
 ENTRY DATE: Entered STN: 19900308
 Last Updated on STN: 19900308
 Entered Medline: 19880825

ED Entered STN: 19900308
 Last Updated on STN: 19900308
 Entered Medline: 19880825

AB Two unidentified analytical responses in a papaya extract were structurally determined by mass spectrometry to be benzyl isothiocyanate and phenyl acetonitrile. Both these compounds have previously been shown to result from degradation of benzylglucosinolate that occurs naturally in the seeds of the fruit. Characterization by mass spectrometry has now provided a convenient mechanism to detect both these degradation compounds in extracts resulting from routine pesticide residue analysis.

L47 ANSWER 8 OF 8 MEDLINE on STN
 ACCESSION NUMBER: 86180719 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 3961819
 TITLE: Glutathione- and cysteine-mediated cytotoxicity of allyl and benzyl isothiocyanate.
 AUTHOR: Bruggeman I M; Temmink J H; van Bladeren P J
 SOURCE: Toxicology and applied pharmacology, (1986 Apr) 83 (2) 349-59.
 Journal code: 0416575. ISSN: 0041-008X.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 198604
 ENTRY DATE: Entered STN: 19900321
 Last Updated on STN: 20000303
 Entered Medline: 19860430
 ED Entered STN: 19900321
 Last Updated on STN: 20000303
 Entered Medline: 19860430
 AB Allyl isothiocyanate has been reported to be a bladder carcinogen in male rats. On the other hand, benzyl isothiocyanate is an anti-carcinogen. These contradicting properties led us to investigate the cytotoxicity of these compounds in RL-4 rat hepatocytes. Since conjugation with glutathione plays an important role in the metabolism of these isothiocyanates, the glutathione and L-cysteine derivatives were also tested for cytotoxicity (electron microscopy, trypan blue exclusion, cell attachment, and inhibition of cell division). Both types of conjugates caused considerable toxicity: allyl isothiocyanate conjugates gave effects comparable to the parent compound, but benzyl isothiocyanate was more toxic than its conjugates. Addition of excess glutathione (greater than 4mM) to the free isothiocyanates as well as their conjugates abolished cytotoxicity up to the highest concentration tested (250 micromM). Addition of excess L-cysteine (5 to 20 mM) lowered the effects but did not abolish them. The reaction of thiols with isothiocyanates was readily reversible: 15 min after dissolving the conjugates in buffer, pH 7.4, an equilibrium was established in which 9 to 15% of the conjugates was converted to free isothiocyanate. Two hours after addition of 1 mM of the L-cysteine conjugates to medium containing 5 mM glutathione, 80% of the total conjugates was present as the glutathione derivatives. The glutathione conjugates were similarly converted to L-cysteine conjugates. Glutathione conjugates are not able to enter the cell, thus their toxicity is presumably due to the release of free isothiocyanate, and in the presence of excess glutathione no toxicity was observed. L-cysteine derivatives are able to cross the cell membrane, thus excess L-cysteine diminishes cytotoxicity, since less free isothiocyanate is present outside the cells, but does not completely protect the cells. Glutathione and cysteine can be regarded as transporting agents for the isothiocyanates through the body. Initial detoxification can be followed by release of the reactive compound at some other site.

=> fil hom

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FILE 'HOME' ENTERED AT 12:35:27 ON 24 JUN 2004

Searcher : Shears 571-272-2528